

Isothiazole, 4-phenyl-

Other names:	4-Phenylisothiazole
Inchi:	InChI=1S/C9H7NS/c1-2-4-8(5-3-1)9-6-10-11-7-9/h1-7H
InchiKey:	RAUUYMXHIUAZCW-UHFFFAOYSA-N
Formula:	C9H7NS
SMILES:	<chem>c1ccc(-c2cncs2)cc1</chem>
Mol. weight [g/mol]:	161.22
CAS:	936-46-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.60		Crippen Method
logp	2.810		Crippen Method
mcvol	120.780	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C936469&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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